Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

Model Results

Predicted value: 3.98e-02 mol/L

Global applicability domain: Inside

Local applicability domain index: 4.05e-01

Confidence level: 5.80e-01

Nearest Neighbors from the Training Set

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Psicofuranine
Measured: 2.69e-02
Predicted: 3.98e-02

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Inosine
Measured: 5.89e-02
Predicted: 6.83e-02

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Ribavirin
Measured: 5.81e-01
Predicted: 1.18e-01

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Idoxuridine
Measured: 5.65e-03
Predicted: 9.97e-03